



# Workshop Goals & Process

Large Scale Computing and Storage Requirements  
for Fusion Energy Sciences

Joint FES / ASCR / NERSC Workshop

August 3-4, 2010





# Logistics: Schedule

- Agenda on workshop web page
  - [http://www.nersc.gov/projects/science\\_requirements/FES/agenda.php](http://www.nersc.gov/projects/science_requirements/FES/agenda.php)
- Mid-morning / afternoon break, lunch
- Self-organization for dinner
- 9 “science areas,” one workshop
  - Science-focused but cross-science discussion
  - Explore areas of common need (within FES)
- Breakout sessions Weds AM



# Why is NERSC Collecting Computational Requirements?

- Help ASCR and NERSC make informed decisions for technology and services.
- Input is used to guide procurements, staffing, and to improve the effectiveness of NERSC services.
  - Includes hardware, software, support, data, storage, analysis, work flow
  - Time frame: 2014
- Result: NERSC can better provide what you need for your work.



# Logistics: Case Studies

- One co-lead (for each science area)
  - help roll up discussions into major case studies
- Case Studies:
  - Narrative describing science & NERSC reqmts
  - Audience is NERSC, DOE program managers
  - Initial set suggested by John Mandrekas
    - Minimum set to capture FES mission and unique NERSC requirements
  - Encourage participation by all; roundtable



# Logistics: Worksheets

- Web Worksheets: “Reference Material”
  - Based on NERSC info
  - Summary of projects as we know them
  - Good point of departure
    - A framework for discussion
    - But not necessarily the entire story



# Logistics: Final Report Content

- Format similar to ESnet
  - But NERSC requirement space much broader than Esnet
  - See “Reference Material” on web site
  - Contents
    - Executive summary,
    - ~2-page case study reports,
    - NERSC synthesis of all results



# Logistics: Final Report Schedule

- Case studies due to NERSC ..... Aug 27
- NERSC draft report ..... Oct 1
- Participants review period ..... Oct 22
- NERSC Near final ..... Nov 5
- BES AD approval .....
- NERSC Revisions .....
- Final Report posted on Workshop Webpage



# Examples of Information Sought

- Type of simulation, #, reason for #, algorithms, solver
- Parallelism: method, weak or strong scaling, implementation, concurrency, limits
- Key physical parameters and their limits:
  - spatial resolution, # of atoms/energy levels, integration range, ...
- Representative code
- Key science result metrics and goals



# Examples of Information Sought

- Typical science process (workflow)
- Data: amount stored / transferred for input, results, and fault mitigation
- Special needs for data intensive projects
  - Grids, gateways, workflows, provenance, `
- Special query regarding multicore/manycore
  
- How all of this is
  - Driven by the science
  - Likely to change and why



# Final Thoughts

- Requirements characterization process is not complicated.
- Mutually beneficial.

# Scaling Science

Inspired by **P. Kent**,  
“*Computational Challenges in  
Nanoscience: an ab initio  
Perspective*”, Peta08 workshop,  
Hawaii (2008) and **Jonathan  
Carter** (NERSC).

**Convergence,  
systematic errors  
due to cutoffs, etc.**

**Length, Spatial  
extent, #Atoms, *Weak  
scaling***

**Time scale  
Optimizations, *Strong  
scaling***

**Initial Conditions, e.g.  
molecule,  
boundaries,  
*Ensembles***

**Simulation method,  
e.g. DFT, QMC or HF/  
SCF; LES or DNS**